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TITLE

Simple Polynomial Fittings for Steam

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ABSTRACT

The purpose of this report is to develop fittings for saturation curve, steam density and its derivatives to be used in FINFLO Navier-Stokes solver in two-phase flow computations.

MAIN RESULT

A flexible method to fit data

PAGES

13

KEY WORDS

FINFLO, steam density fitting, derivatives of density

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Abstract

This report presents a new flexible method to define piecewise polynomial fittings for data that is a function of two variables. The accuracy can be easily improved by adding new polynomes into the old polynome group. The method is applied to obtain fittings for steam density on the range 273.16-600 K and 0-2 MPa and saturation curve on the range varying between the triple and the critical points. The polynomes are utilised to compute the derivatives of the density. The fittings are compared with the steam table values.

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Nomenclature

A	auxiliar variable
f	component of weighting function
F	weighting function
T	temperature
p	pressure
ρ	density

Subscripts

$crit$	critical point
f	fitting
i	index
low	lower value
sat	saturation
t	table
$trip$	triple point
up	upper value

1 Introduction

Multi-phase computations need material data for each phase and data when the phase-change occurs. Data is usually given using polynomial fittings. This report contains some fittings presented in a flexible way for FINFLO Navier-Stokes solver. The steam density on the range 273.16-573.16 K and 0-300 kPa and the saturation curve between the triple and the critical points are presented. Derivatives of steam density can be computed explicitly. The prefixed accuracy for the density is some percents and for the derivatives about 10 percents. Later the accuracy can be improved easily in any region where it is necessary by adding more polynomes beside the old ones.

2 Fittings

The fittings are as simple as possible within desired accuracy. The polynoms are computationally the cheapest ones but they are not always accurate enough. The next chapters present the fittings for saturation curve and steam density.

2.1 Saturation curve $p_{sat}(T_{sat})$ and $T_{sat}(p_{sat})$

Any polynomial function for $p_{sat}(T_{sat})$ to fit the whole region from the triple point to the critical point becomes too complicated to compute. The next logarithmic formula fits quite well in the whole region

$$\ln\left(\frac{p_{sat}}{p_{crit}}\right) = \frac{1 - (T_{crit}/T_{sat})}{1 - (T_{crit}/T_{trip})} \ln\left(\frac{p_{trip}}{p_{crit}}\right) \quad (1)$$

$$p_{sat} = p_{crit} \left(\frac{p_{trip}}{p_{crit}}\right)^A \quad (2)$$

$$A = \frac{1 - (T_{crit}/T_{sat})}{1 - (T_{crit}/T_{trip})} \quad (3)$$

where the triple and critical point values are $T_{trip}=273.16$ K, $p_{trip}=611.65$ Pa, $T_{crit}=647.10$ K and $p_{crit}=22.064$ MPa. This can be solved for the saturation temperature as

$$T_{sat} = \frac{T_{crit}}{1 - \left(1 - \frac{T_{crit}}{T_{trip}}\right) \frac{\ln\left(\frac{p_{sat}}{p_{crit}}\right)}{\ln\left(\frac{p_{trip}}{p_{crit}}\right)}} \quad (4)$$

The previous formula type can be used to create a composite function which fits better in certain regions. The basic idea is to adjust the lower and upper values for T and p for each region.

$$\ln\left(\frac{p_{sat}}{p_{up}}\right) = \frac{1 - (T_{up}/T_{sat})}{1 - (T_{up}/T_{low})} \ln\left(\frac{p_{low}}{p_{up}}\right) \quad (5)$$

$$p_{sat} = p_{up} \left(\frac{p_{low}}{p_{up}} \right)^A \quad (6)$$

Consequently, the saturation temperature can be written

$$A = \frac{1 - (T_{up}/T_{sat})}{1 - (T_{up}/T_{low})} \quad (7)$$

$$T_{sat} = \frac{T_{up}}{1 - \left(1 - \frac{T_{up}}{T_{low}}\right) \frac{\ln\left(\frac{p_{sat}}{p_{up}}\right)}{\ln\left(\frac{p_{low}}{p_{up}}\right)}} \quad (8)$$

It is not necessary to use the same values as the upper limit of a previous region and a lower one of the next region. The matching is executed with piecewise linear weighting functions F_1 and F_2 which work in a certain region $T_1 \leq T \leq T_2$ around the limits. Elsewhere the unit weighting is used, e.g. f_0 and f_3 . The functions for a composite of two parts is written

$$F_1 = \text{MAX}[0., \text{MIN}[f_0, f_1]] \quad (9)$$

$$F_2 = \text{MAX}[0., \text{MIN}[f_2, f_3]] \quad (10)$$

where

$$f_0 = 1. \quad (11)$$

$$f_1 = \frac{T_2 - T}{T_2 - T_1} \quad (12)$$

$$f_2 = \frac{T - T_1}{T_2 - T_1} \quad (13)$$

$$f_3 = 1. \quad (14)$$

which are illustrated in the next figure.

Figures 2 and 3 present the fitting which contains two logarithmic parts, $T_{low,1} = T_{trip}$, $T_{up,1}=343.16$ K, $T_{low,2}=373.16$ K and $T_{up,2} = T_{crit}$. The corresponding pressures are $p_{low,1} = p_{trip}$, $p_{up,1}=31176$ Pa, $p_{low,2}=101320$ Pa and $p_{up,2} = p_{crit}$. The switching off and on of the previous logarithmic functions are executed linearly in the region $353.16 \text{ K} \leq T \leq 363.16 \text{ K}$.

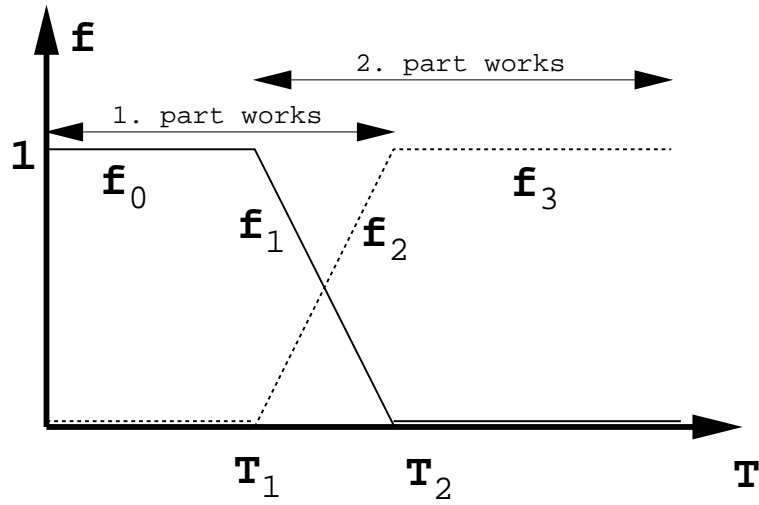


Fig. 1: The linear weighting functions switching off and on the fittings.

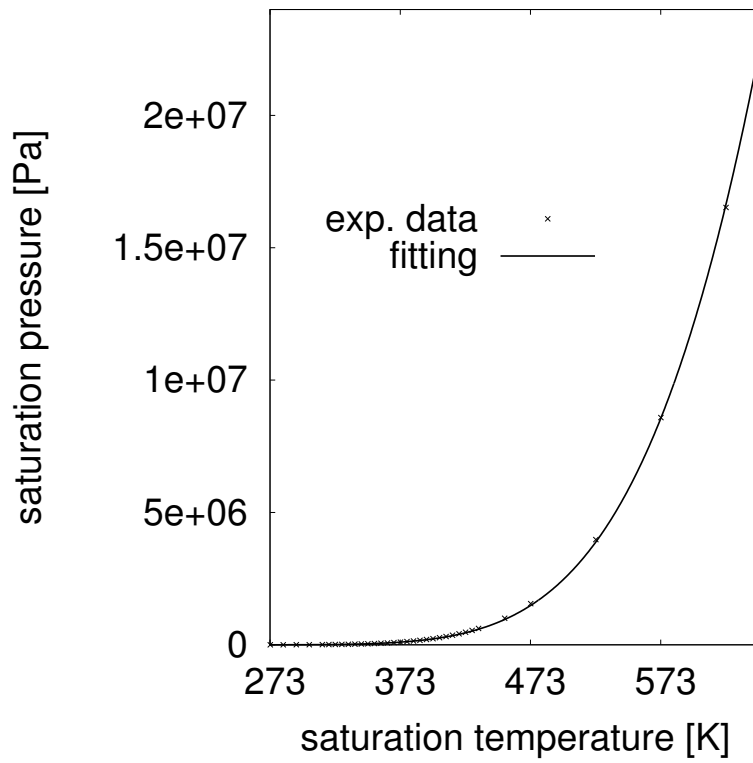


Fig. 2: Saturation pressure as a function of saturation temperature from the triple to the critical point.

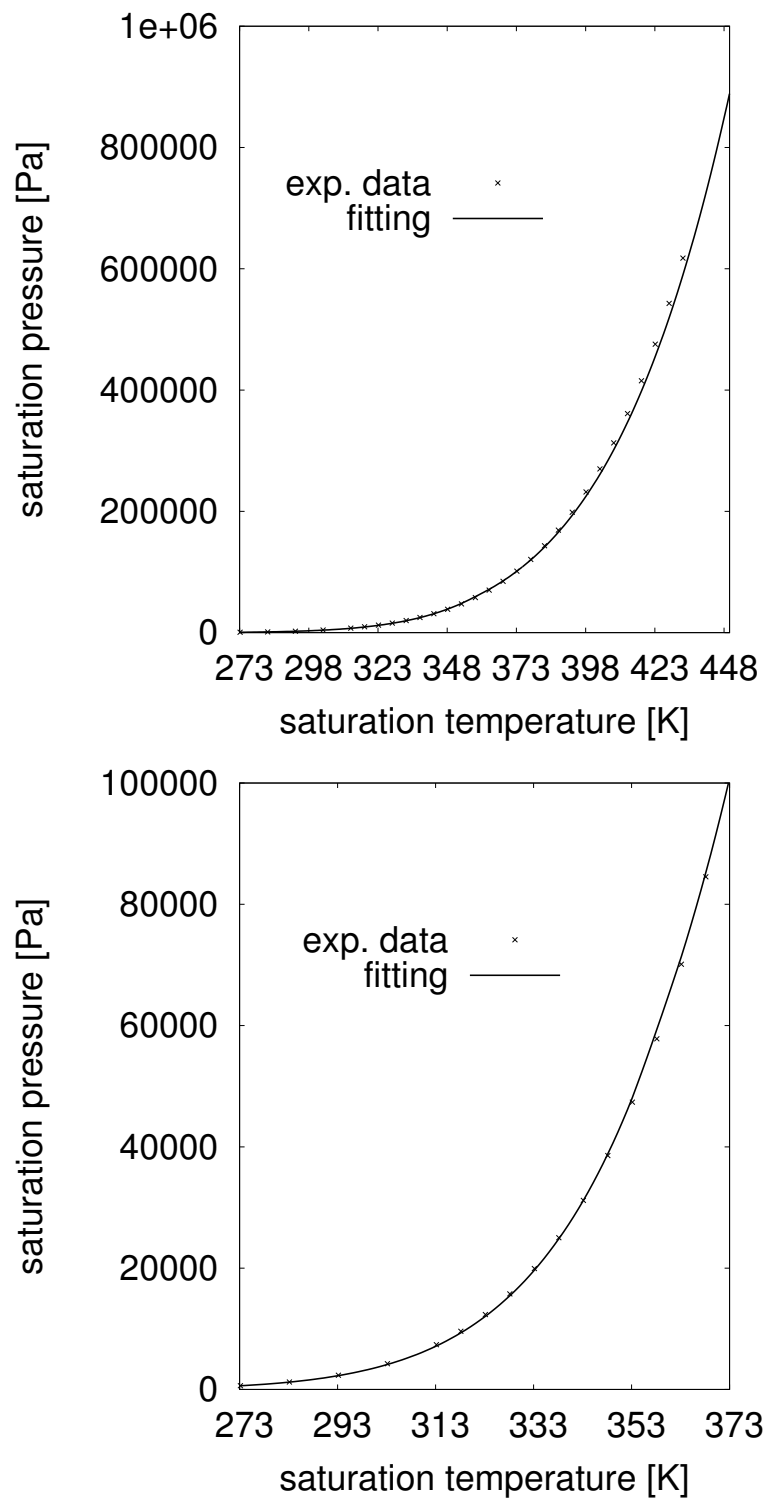


Fig. 3: Saturation pressure as a function of saturation temperature near the triple point.

2.2 Fitting for steam density $\rho(T, p)$

A simple and an accurate enough fitting for steam density $\rho(T, p)$ is achieved by using second-order polynome $\rho_i(T)$ formulas at a fixed pressure. The formulas are connected linearly with respect to the pressure. The linear pressure depending components of the weighting function are like

$$f_{i,0}(p) = 0 \quad (15)$$

$$f_{i,1}(p) = \frac{p}{p_i - p_{i-1}} - \frac{p_{i-1}}{p_i - p_{i-1}} \quad (16)$$

$$f_{i,2}(p) = -\frac{p}{p_{i+1} - p_i} + \frac{p_{i+1}}{p_{i+1} - p_i} \quad (17)$$

$$f_{i,3}(p) = 0 \quad (18)$$

$$F_i(p) = \text{MAX}[0., \text{MIN}[f_{i,1}(p), f_{i,2}(p)]] \quad (19)$$

As the next figure shows the weighting outside the fitted pressure region is unit and the border pressure is used.

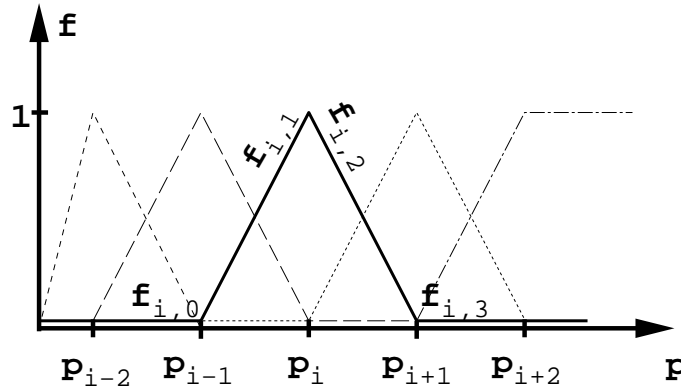


Fig. 4: The linear weighting functions switching off and on the $\rho_i(T)$ fittings.

The second-order polynomial functions are used for $\rho_i(T)$ at pressures 1, 10, 100, 300, 2000 kPa, which are

$$\rho_1(T) = 0.0165018 - 0.0000406131 \times T + 3.22363 \times 10^{-8} \times T^2 \quad (20)$$

$$\rho_{10}(T) = 0.156294 - 0.00036745 \times T + 2.81416 \times 10^{-7} \times T^2 \quad (21)$$

$$\rho_{100}(T) = 1.49104 - 0.00331947 \times T + 2.40937 \times 10^{-6} \times T^2 \quad (22)$$

$$\rho_{300}(T) = 4.57358 - 0.0101508 \times T + 7.26955 \times 10^{-6} \times T^2 \quad (23)$$

$$\rho_{2000}(T) = 30.1263 - 0.0585389 \times T + 0.0000348933 \times T^2 \quad (24)$$

and the final formula of the density is written

$$\rho(T, p) = \sum_i F_i(p) \rho_i(T) \quad (25)$$

The steam density fitting is continuous which is important from the numerical point of view. The continuity of the formulas can be seen in Figures 5-12. The steam table values are from Haar et al. [1] and Keenan et al. [2].

The fitting works very accurately in the region $p=0-300$ kPa and $T=273.16-573.16$ K. At the pressure of 400 kPa the error is about 2.5% increasing as the pressure increases. The fitting pressure 2 MPa is used to keep the density within adequate values even if the subroutine is called with inadequate temperature and pressure values. In subcooled region the density gets proper values as in high temperature values. Rather the temperature and pressure values are required to be limited to prevent more general damages during the iteration than the fitting begins to fail irresponsibly.

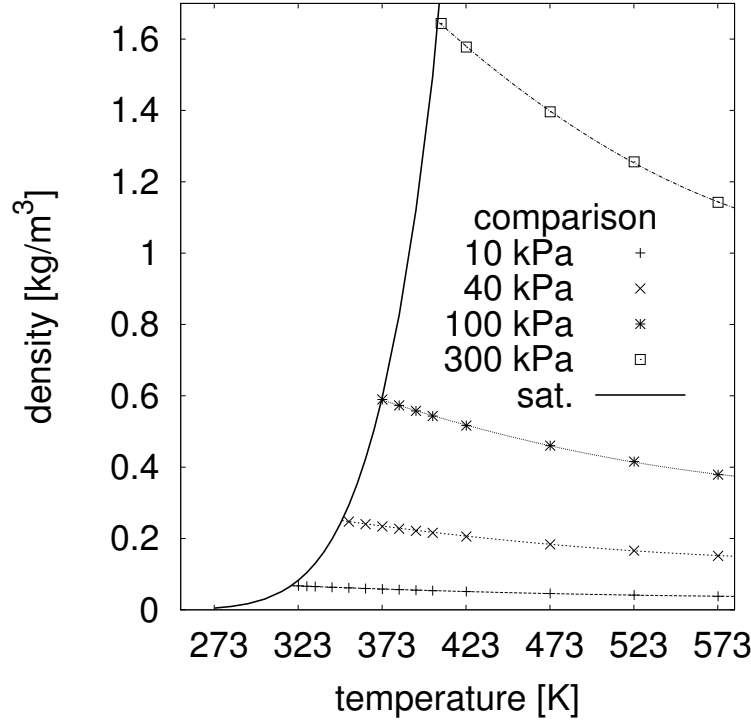


Fig. 5: Density as function of T .

The derivatives of the density $\partial\rho/\partial T|_p$ and $\partial\rho/\partial p|_T$ are computed straightly using the previous fitting. The derivatives of the $\rho_i(T)$ components are

$$\rho_1(T) = -0.0000406131 + 6.44726 \times 10^{-8} \times T \quad (26)$$

$$\rho_{10}(T) = -0.00036745 + 5.62832 \times 10^{-7} \times T \quad (27)$$

$$\rho_{100}(T) = -0.00331947 + 4.81874 \times 10^{-6} \times T \quad (28)$$

$$\rho_{300}(T) = -0.0101508 + 1.45391 \times 10^{-5} \times T \quad (29)$$

$$\rho_{2000}(T) = -0.0585389 + 0.000069787 \times T \quad (30)$$

A straightforward computation of $\partial\rho/\partial p|_T$ gives errors that may cause problems. The values seem to contain even 20-30% error and the linear pressure

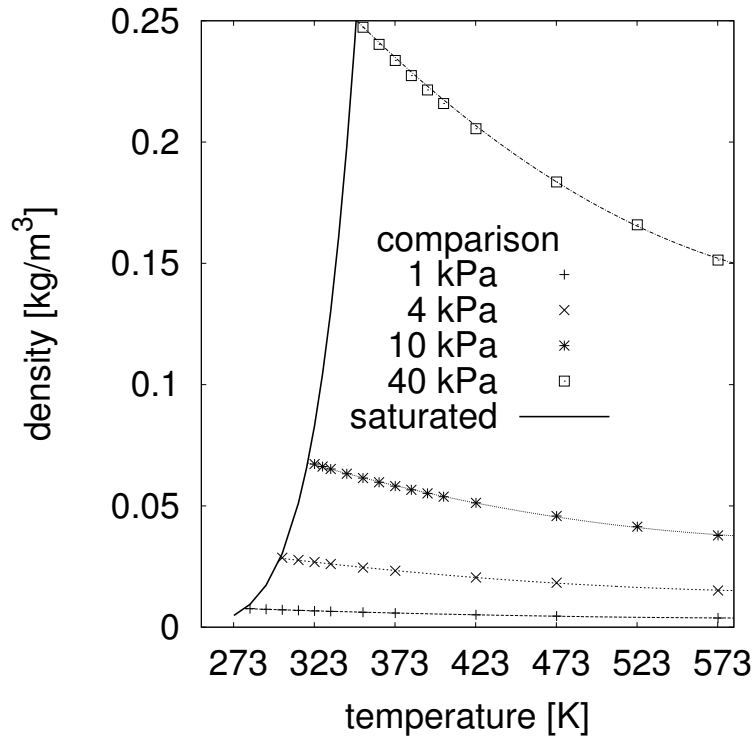


Fig. 6: Density as function of T .

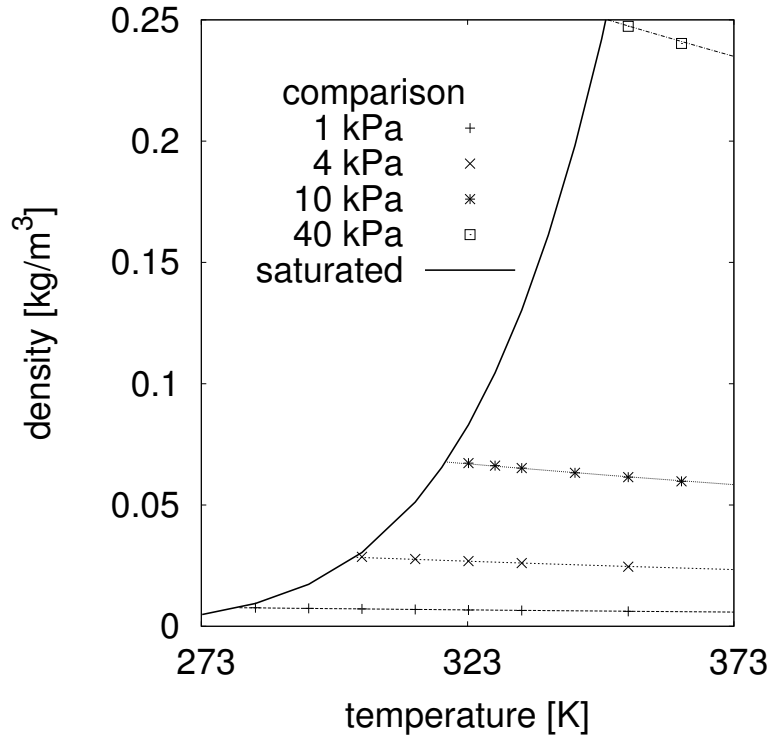


Fig. 7: Density as function of T .

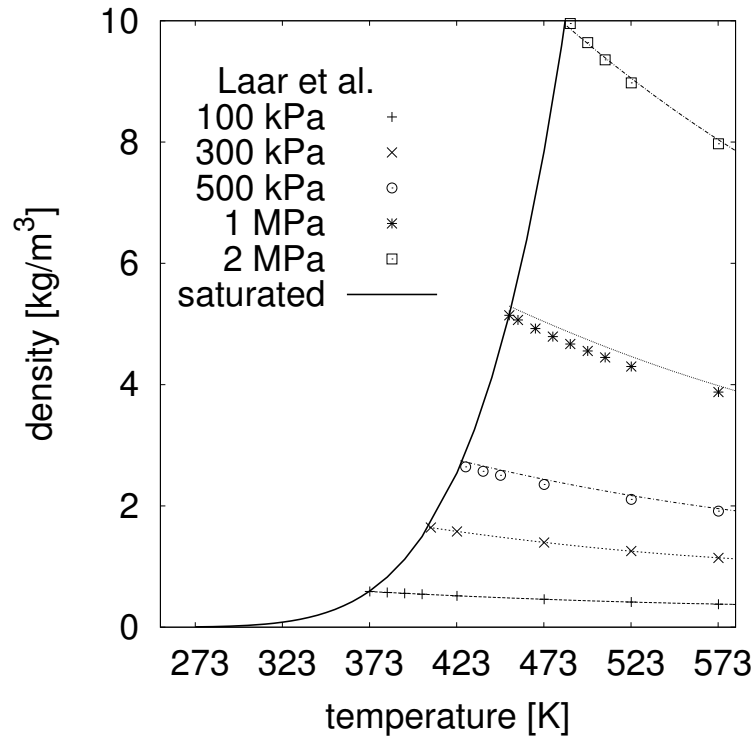


Fig. 8: Density as function of T .

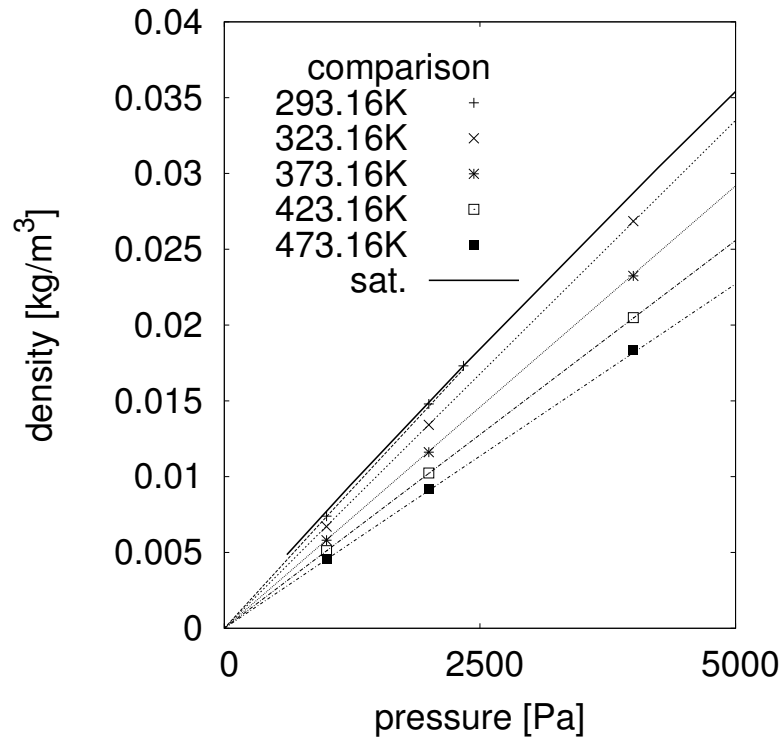


Fig. 9: Density as function of p .

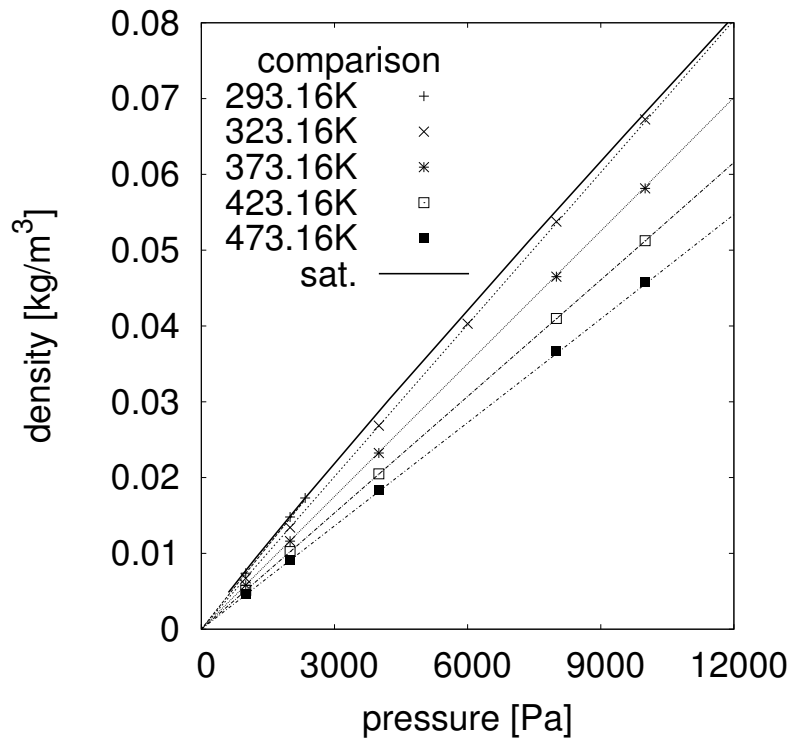


Fig. 10: Density as function of p .

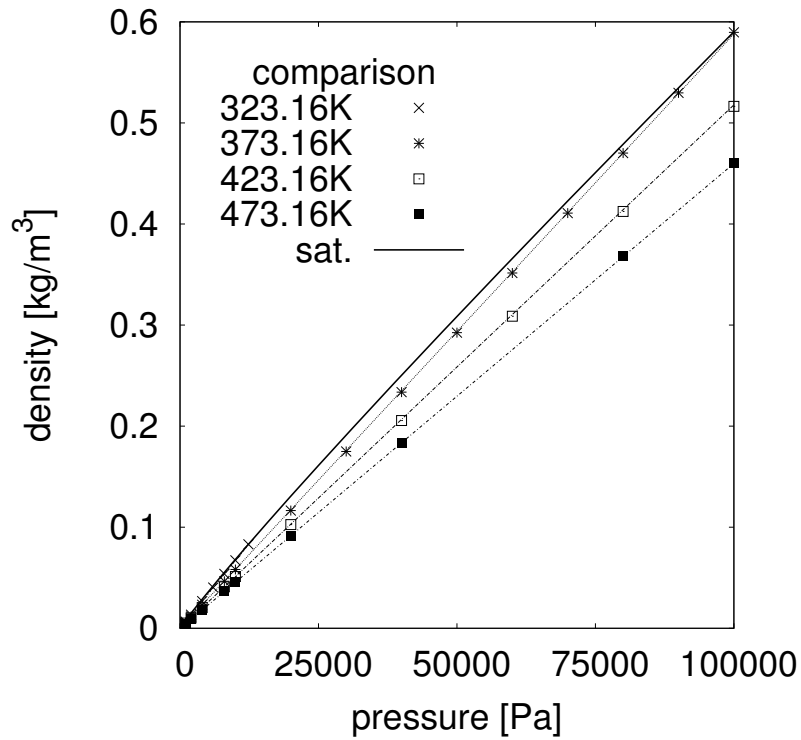


Fig. 11: Density as function of p .

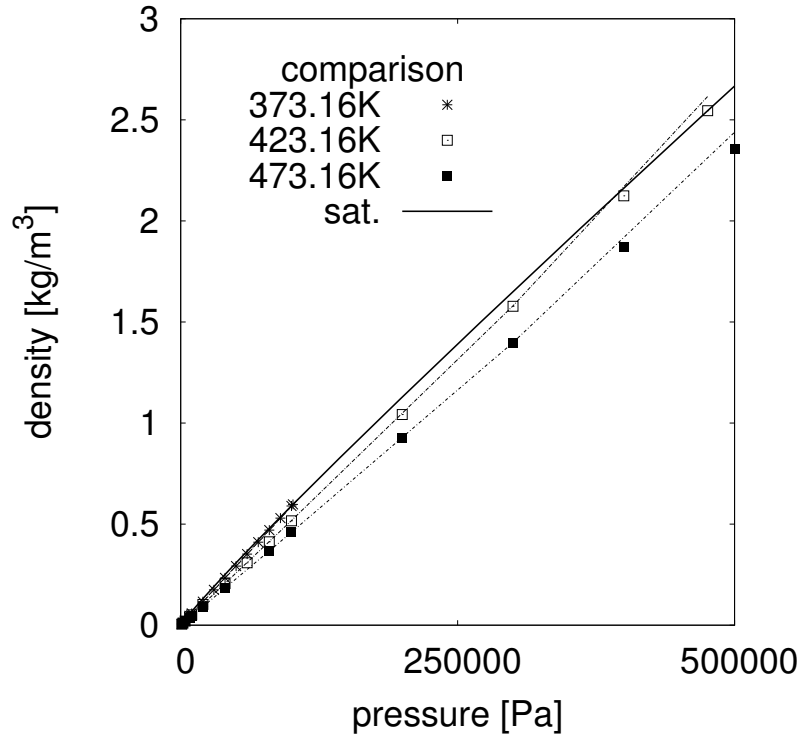


Fig. 12: Density as function of p .

dependence of the density cause discontinuous derivative values. Furthermore, the formula becomes quite long. Therefore, a very simple and accurate method to compute the $\partial\rho/\partial p|_T$ is suggested

$$\left.\frac{\partial\rho}{\partial p}\right|_T \approx \frac{\rho}{p} \quad (31)$$

where the absolute pressure must be used. The acceptance for the approximation can be observed from the figures of the density as function of pressure. The comparison of the formula (31) with the table values gives surprisingly accurate results. It must be kept in mind that the table values do not contain data enough to compute the derivatives with a particular accuracy.

The next table presents some density values compared with the table values. The largest errors can be found when the pressure is about 10 MPa because the $\rho_i(T)$ fittings are used for the pressures 300 kPa and 20 MPa. The accuracy could be improved by adding a new fitting for the pressure 10 MPa.

T	p	ρ_f	ρ_t
323.1600	10000.00	0.066937804	0.06725
343.1600	10000.00	0.063339062	0.06328
363.1600	50000.00	0.3014481	0.30088
393.1600	50000.00	0.2789084	0.27717
473.1600	50000.00	0.2296017	0.22957
423.1600	80000.00	0.4141143	0.41242
373.1600	100000.0	0.5878474	0.58960
573.1600	100000.0	0.3799604	0.37896
398.1600	200000.0	1.117855	1.1138
473.1600	200000.0	0.9289735	0.9257
408.1600	300000.0	1.641497	1.6438
473.1600	300000.0	1.398137	1.3962
573.1600	300000.0	1.143684	1.1425
673.1600	300000.0	1.034623	0.9694
473.1600	400000.0	1.918240	1.8721
473.1600	500000.0	2.438348	2.3537
453.1600	1000000.	5.294983	5.1432
523.1600	1000000.	4.463891	4.2984
488.1600	2000000.	9.865028	9.954
523.1600	2000000.	9.051258	8.976
573.1600	2000000.	8.037024	7.971
673.1600	2000000.	6.531956	6.614

3 Conclusions

It was found that the saturation curve is quite impossible to fit without a logarithmic function. The saturation curve was cut into two parts to improve the accuracy and the parts were connected with linear weighting functions.

The steam density formula was constructed using a group of $\rho_i(T)$ fittings which were connected with linear pressure weighting functions. The accuracy of density is within a few percent in the design region $T=273.16\text{-}573.16$ K and $p=0\text{-}300$ kPa. The derivative $\partial\rho/\partial T|_P$ can be computed explicitly but the $\partial\rho/\partial p|_T$ is not accurate enough and it contains discontinuities. The formula $\partial\rho/\partial p|_T \approx \rho/p$ seems to work nicely.

In general, the presented piecewise fitting method gives quite accurate results, and the accuracy can be improved easily by adding more polynomes in the regions where improved accuracy is needed.

References

- [1] Haar, L., Gallagher, J., and Kell, G., *NBS/NRC Steam Tables, Thermodynamic and Transport Properties and Computer Programs for Vapor and Liquid States of Water in SI Units*. Washington: Hemisphere Publishing Corporation, 1984. ISBN 0-89116-353-0.
- [2] Keenan, J., Keyes, F., Hill, P., and Moore, J., *Steam Tables (S.I. Units)*. New York: John Wiley & Sons, 1978. ISBN 0-471-04210-2.